



FORM PTO-1489 (Modified)

LIST OF PATENTS AND PUBLICATIONS FOR
APPLICANT'S INFORMATION DISCLOSURE
STATEMENTATTY. DOCKET NO.
24737-1906BSERIAL NO.
09/704,362APPLICANT
Ramnarayan *et al.*FILING DATE
November 1, 2000GROUP
~~2857~~
1631

TECH CENTER 1600/2900

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL	DOCUMENT NUMBER	DATE	NAME	CLASS	SUB CLASS	FILING DATE

FOREIGN PATENT DOCUMENTS

	DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB CLASS	Translation	
						Yes	No
<i>pb</i>	0 1 3 5 3 1 6	05/17/01	PCT				

OTHER ART (Including Author, Title, Date, Pertinent Pages, Etc.)

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J. B. Bruce

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FORM PTO-1449 (Modified)

ATTY. DOCKET NO.
24737-1906B

SERIAL NO.
09/704,362

LIST OF PATENTS AND PUBLICATIONS FOR
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APPLICANT
Ramnarayan *et al.*

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER							DATE	NAME	CLASS	SUB CLASS	FILING DATE
JB	AA	5	3	3	1	5	7	3	07/19/94	Balaji <i>et al.</i>	364	500	12/14/90
JB	AB	5	5	7	9	2	5	0	11/26/96	Balaji <i>et al.</i>	364	496	04/24/95
JB	AC	5	6	1	2	8	9	5	03/18/97	Balaji <i>et al.</i>	364	496	04/21/95
JB	AD	5	8	0	8	6	9	9	09/15/98	Arnaud <i>et al.</i>	367	103	12/04/95
JB	AE	5	8	3	7	4	6	4	11/17/98	Capon <i>et al.</i>	435	6	01/29/97
JB	AF	5	8	4	6	7	6	3	12/08/98	Lee <i>et al.</i>	435	69.1	05/13/94
JB	AG	5	9	1	0	4	8	8	06/08/99	Hlavka <i>et al.</i>	514	9	09/20/96

FOREIGN PATENT DOCUMENTS

		DOCUMENT NUMBER							DATE	COUNTRY	CLASS	SUB CLASS	Translation Yes No	
JB	AH	0	5	3	3	0	9	3	09/28/00	PCT				
JB	AI	9	5	0	6	2	9	3	03/02/95	PCT				
JB	AJ	9	5	1	4	0	2	8	05/26/95	PCT				
JB	AK	9	5	1	4	0	2	8	07/31/97	PCT				
JB	AL	9	5	1	4	0	2	8	07/31/97	PCT				
JB	AM	9	8	0	6	0	4	8	02/12/98	PCT				
JB	AN	9	8	1	3	7	8	1	04/02/98	PCT				
JB	AO	9	8	5	4	6	6	5	12/03/98	PCT				
JB	AP	9	9	0	6	5	9	7	02/11/99	PCT				

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Title: **USE OF COMPUTATIONALLY DERIVED PROTEIN STRUCTURES OF GENETIC
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FORM PTO-1449 (Modified) LIST OF PATENTS AND PUBLICATIONS FOR APPLICANT'S INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 24737-1906B	SERIAL NO. 09/704,362
	APPLICANT Ramnarayan <i>et al.</i>	
	FILING DATE November 01, 2000	GROUP 2857 /63/

OTHER ART (Including Author, Title, Date, Pertinent Pages, Etc.)

JB	AQ	Abagyan <i>et al.</i> "Biased Probability Monte Carlo Conformational Searches and Electrostatic Calculations for Peptides and Proteins," <i>J. Mol. Biol.</i> <u>235</u> : 983-1002 (1994).
JB	AR	Abdel-Meguid, S.S. <i>et al.</i> "An orally bioavailable HIV-1 protease inhibitor containing an imidazole-derived peptide bond replacement: crystallographic and pharmacokinetic analysis," <i>Biochemistry</i> 33(39):11671-11677 (1994)
JB	AS	Altschul <i>et al.</i> "Basic Local Alignment Search Tool," <i>J. Mol. Biol.</i> <u>215</u> : 403-10 (1990).
JB	AT	Balasubramanian, R., "New type of representation for mapping chain-folding in protein molecules," <i>Biopolymers</i> <u>26</u> : 856-57 (1977).
JB	AU	Blaney, R. "Molecular modelling in the pharmaceutical industry," <i>Chemistry and Industry. Chemistry and Industry Review</i> 23(4):791-4 (1990).
not considered	AV	Biocomputing: Informatics and Genome Projects Smith, D.W., ed. Academic Press, Inc., San Diego (1994). <i>no copy provided</i>
JB	AW	Bohm, G. "New approaches in molecular structure prediction" <i>Biophysical Chemistry</i> 59:1-32 (1996)
JB	AX	Bouas <i>et al.</i> "Design, Synthesis, and Evaluation of Conformationally Constrained Tongs, New Inhibitors of HIV-1 Protease Dimerization," <i>J. Med. Chem.</i> <u>42</u> : 957-62 (1999).
JB	AY	Carrillo, H. and D. Lipman., "The Multiple Sequence Alignment Problem in Biology," <i>SIAM J. Appl. Math.</i> <u>48</u> (5): 1073-82 (1988).
not considered	AZ	Computational Molecular Biology: Sources and Methods for Sequence Analysis Lesky A.M., ed. Oxford University Press, New York (1988) <i>no copy provided</i>
JB	BA	Devereux <i>et al.</i> "A comprehensive set of sequence analysis programs for the VAX," <i>nucl. Acids Res.</i> <u>12</u> (1): 387-95 (1984).
not considered	BB	Dialog #03523908 JICST Acc. No.: 98A0122627 English language description of Habuka, Noriyaki, "Crystal structure of HCV NS3 protease," <i>Jikken Igaku</i> <u>15</u> (19): 2308-13 (1997). <i>no translation or statement of relevance</i>
JB	BC	Dudek <i>et al.</i> "Protein Structure Prediction Using a Combination of Sequence Homology and Global Energy Minimization: II. Energy Functions," <i>Journal Computational Chemistry</i> <u>19</u> : 548-73 (1998).
JB	BD	Goodeell, D.S. and A. J. Olson, "Automated Docking of Substrates to Proteins by Simulated Annealing," <i>Proteins: Structure Function, and Genetics</i> <u>8</u> : 195-202 (1990).

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Title: **USE OF COMPUTATIONALLY DERIVED PROTEIN STRUCTURES OF GENETIC POLYMORPHISMS IN PHARMACOGENOMICS FOR DRUG DESIGN AND CLINICAL APPLICATIONS**

FORM PTO-1449 (Modified)	ATTY. DOCKET NO. 24737-1906B	SERIAL NO. 09/704,362	RECEIVED MAR 21 2002 TECH CENTER 1600/2900
	APPLICANT Ramnarayan <i>et al.</i>		
	FILING DATE November 01, 2000	GROUP 2857/631	

LIST OF PATENTS AND PUBLICATIONS FOR
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STATEMENT

OTHER ART (Including Author, Title, Date, Pertinent Pages, Etc.)

JB	BE	Gribskov, M. and R.R. Burgess., "Sigma factors from <i>E. coli</i> , <i>B. subtilis</i> , phage SP01, and phage T4 are homologous proteins," <i>Nucl. Acids Res.</i> <u>14(1)</u> : 6745-63 (1986).
not considered	BF	Guide to Human Genome Computing Bishop, M., ed. Academic Press, Inc., San Diego (1994). <i>no copy provided</i>
JB	BG	Gulnik <i>et al.</i> "Kinetic Characterization and Cross-Resistance Patterns of HIV-1 Protease Mutants Selected under Drug Pressure," <i>Biochemistry</i> <u>35</u> : 9282-7 (1995).
not considered	BH	Habuka <i>et al.</i> "Crystal Structure of HCV NS3 protease," <i>Jikken Igaku</i> <u>15(19)</u>: 2308-13 (1997). <i>no translation or statement of relevance</i>
JB	BI	Jacobsen <i>et al.</i> "Characterization of Human Immunodeficiency Virus Type 1 Mutants with Decreased Sensitivity to Protease Inhibitor Ro 31-8959," <i>Virology</i> <u>206</u> : 527-34 (1995).
JB	BJ	Kim <i>et al.</i> "Crystal Structure of the Hepatitis C virus Ns3 Protease Domain complexed with a Synthetic NS4A Cofactor Peptide," <i>Cell</i> <u>87</u> : 343-355 (1996).
JB	BK	Klabe <i>et al.</i> "Resistance to HIV Protease Inhibitors: a Comparison of Enzyme Inhibition and Antiviral Potency," <i>Biochemistry</i> <u>37</u> : 8735-42 (1998).
JB	BL	Kohlstaedt <i>et al.</i> "Crystal Structure at 3.5 Angstrom Resolution of HIV-1 Reverse Transcriptase Complexed with an Inhibitor," <i>Science</i> <u>256</u> : 1783-1790 (1992).
	BM	Kroeger <i>et al.</i> "Molecular modeling of HIV-1 reverse transcriptase drug-resistant mutant strains; implications for the mechanism of polymerase action," <i>Protein Engineering</i> <u>10(12)</u> : 1379-1383 (1997).
	BN	Kuntz <i>et al.</i> "Structure-Based Strategies for Drug Design and Discovery," <i>Science</i> <u>257</u> : 1078-82 (1992).
	BO	Kuntz <i>et al.</i> "A Geometric Approach to Macromolecule-Ligand Interactions," <i>J. Mol. Biol.</i> <u>161</u> : 269-288 (1982).
	BP	Lambert, M., "Docking Conformationally Flexible Molecules into Protein Binding Sites," in <i>Practical Application of Computer-Aided Drug Design</i> , Charifson, ed. Marcel Dekker, NY, pp.243-303. (1997).
↓	BQ	Maschera <i>et al.</i> "Human Immunodeficiency Virus," <i>J. Biol. Chem.</i> <u>271(52)</u> : 33231-5 (1996). <i>N/</i>
not considered	BR	Methods in Molecular Biology vol. 24; Computer Analysis of Sequence Data, Part 1. Griffin, A. and H.G. Griffin, eds. Humana Press, Inc. Totowa, New Jersey (1994). <i>no copy provided</i>

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J.B. Brusca

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	APPLICANT Ramnarayan <i>et al.</i>	
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OTHER ART (Including Author, Title, Date, Pertinent Pages, Etc.)

JB	BD	Momany <i>et al.</i> "Energy Parameters in Polypeptides. VII. Geometric Parameters, Partial Atomic Charges, Nonbonded Interactions, Hydrogen Bond Interactions, and Intrinsic Torsional Potentials for the Naturally Occurring Amino Acids," <i>The Journal of Physical Chemistry</i> <u>79</u> (22): 2361-81 (1975).
JB	BT	Murcko, M.A., "An Introduction to De Novo Ligand Design," in <i>Practical Application of Computer-Aided Drug Design</i> , Charifson, ed. Mercel Dekker, NY, pp.305-354. (1997).
	BU	Needleman, S.B. and C.D. Wunsch., "A General Method Applicable to the Search for Similarities in the Amino Acid Sequence of Two Proteins," <i>J. Mol. Biol.</i> <u>48</u> : 443-53 (1970).
	BV	Nemethy <i>et al.</i> "Energy Parameters in Polypeptides. 10. Improved Geometrical Parameters and Nonbonded Interactions for Use in the EEPP/3 Algorithm, with Application to Proline-Containing Peptides," <i>J. Phys. Chem.</i> <u>96</u> : 6472-84 (1992).
	BW	Pazhanisamy <i>et al.</i> "Kinetic Characterization of Human Immunodeficiency Virus Type-1 Protease-resistant Variants," <i>J. Biol. Chem.</i> <u>271</u> (30): 17979-85 (1996).
↓	BX	Pearson, W.R. and D.J. Lipman., "Improved tools for biological comparison," <i>Proc. Natl. Acad. Sci. USA</i> <u>85</u> : 2444-8 (1988).
JB	BY	QSAR and Drug Design: New Developments and Applications T. Fugita, ed. Elsevier Science B.V. (1995) pp.3-81.
JB	BZ	Ramnarayan <i>et al.</i> "The effect of polarization energy on the free energy perturbation calculation," <i>J. Chem. Phys.</i> <u>92</u> (12): 7057-67 (1990).
not considered	CA	Richter, R., "AIDS drugs found to be effective in world's most common HIV strains" January 20, 1999. no place of publication
JB	CB	Schapira <i>et al.</i> "Prediction of the binding energy for small molecules, peptides, and proteins," <i>J. Mol. Recognition</i> <u>12</u> : 177-90 (1999).
JB	CC	Schwartz, R.M. and M.O. Dayhoff., "Matrices for Detecting Distant Relationships," Chapter 23 of: <i>Atlas of Protein Sequence and Structure</i> Dayhoff, M.O. ed. National Biomedical Research Foundation pp.353-8 (1978).
not considered	CD	Sequence Analysis in Molecular Biology: Treasure Trove or Trivial Pursuit von Heijne, G., ed. Academic Press, Inc. San Diego (1987). copy not provided
JB	CE	Shafer <i>et al.</i> "Human Immunodeficiency Virus reverse Transcriptase and Protease Sequence Database," <i>Nucl. Acids Res.</i> <u>27</u> (1): 348-52 (1999).

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JB. Briscoe

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OTHER ART (Including Author, Title, Date, Pertinent Pages, Etc.)

JB	CF	Shafer <i>et al.</i> "Identification of Biased Amino Acid Substitution Patterns in Human Immunodeficiency Virus Type 1 Isolates from Patients Treated with Protease Inhibitors," <i>Journal of Virology</i> 73(7): 6197-6202 (1999).
JB	CG	Shenderovich, <i>et al.</i> , "Structural Pharmacogenetic Approach to the Evaluation of Drug Resistant Mutations and HIV-1 Protease", <i>Journal of Clinical Ligand Assay</i> , 24(2):140-144 (2001)
JB	CH	Shoichet, B.K. and I.D. Kuntz, "Protein docking and Complementarity," <i>J. Mol. Biol.</i> 221: 327-466 (1998)
JB	CI	Shoichet <i>et al.</i> "Structure-Based Discovery of Inhibitors of Thymidylate Synthase," <i>Science</i> 259: 1445-50 (1993).
JB	CJ	Smith, T. F. and M. S. Waterman., "Comparison of Biosequences," <i>Adv. Appl. Math.</i> 2: 482-489 (1981).
JB	CK	Stewart <i>et al.</i> "Automated 3D Docking: Inhibitors of α -Chymotrypsin," <i>Medicinal Chemistry Research</i> 1: 439-443 (1992).
JB	CL	Thompson, S.K. <i>et al.</i> "Rational design, synthesis, and crystallographic analysis of a hydroxyethylene-based HIV-1 protease inhibitor containing a heterocyclic P1'-P2' amide bond isoster," <i>Journal of Medicinal Chemistry</i> 37(19):3100-3107 (1994).
JB	CM	Wang and Kollman, "Computational study of protein specificity: The molecular basis of HIV-1 protease drug resistance", <i>PNAS</i> , 98(26):14937-14942 (2001).
JB	CN	Weiner <i>et al.</i> "An All Atom Force Field for Simulations of Proteins and Nucleic Acids," <i>Journal of Computational Chemistry</i> 7(2): 230-52 (1986).

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Attachment 13
to Paper 72

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL	DOCUMENT NUMBER	DATE	NAME	CLASS	SUB CLASS	FILING DATE
<i>JSB</i>	4 2 0 8 4 7 9	06/17/80	Zuk <i>et al.</i>	435	7	07/14/77
	4 2 2 0 4 5 0	09/02/80	Maggio	22	230	04/05/78
	4 2 3 3 4 0 1	11/11/80	Yoshida <i>et al.</i>	435	7	07/14/77
	4 2 3 3 4 0 2	11/11/80	Maggio <i>et al.</i>	435	7	04/05/78
	4 2 7 7 4 3 7	07/01/81	Maggio	422	61	12/10/79
	4 3 8 5 1 2 6	05/24/83	Chen <i>et al.</i>	436	8	03/19/79
	4 3 9 7 9 5 6	08/09/83	Maggio	436	4	12/10/81
	4 7 8 6 4 7 1	11/22/88	Jones <i>et al.</i>	422	81	10/21/83
	4 7 8 9 6 3 1	12/06/88	Maggio	435	8	02/17/84
	4 8 2 8 9 8 1	05/09/89	Maggio	435	8	08/24/83
	4 8 5 9 6 1 0	08/22/89	Maggio	436	8	09/12/86
	5 0 7 9 1 4 2	01/07/92	Coleman <i>et al.</i>	435	82	01/23/87
	5 2 1 5 8 9 9	06/01/93	Dattagupta	435	6	08/23/90
	5 3 3 1 5 7 3	07/19/94	Balaji <i>et al.</i>	364	500	12/14/90
	5 5 7 1 8 2 1	11/05/96	Chan <i>et al.</i>	514	312	05/20/94
	5 5 7 9 2 5 0	11/26/96	Balaji <i>et al.</i>	364	496	04/24/95
	5 6 1 2 8 9 5	03/18/97	Balaji <i>et al.</i>	364	496	04/21/95
*	5 7 1 2 1 4 5	01/27/98	Houghton <i>et al.</i>	435	219	09/06/96
	5 8 0 8 9 6 9	09/15/98	Arnaud <i>et al.</i>	367	103	12/04/95
	5 8 3 7 4 6 4	11/17/98	Capon <i>et al.</i>	435	6	01/29/97
	5 8 4 6 7 6 3	12/08/98	Lee <i>et al.</i>	435	69.1	05/13/94
	5 9 1 0 4 7 8	06/08/99	Hlavka <i>et al.</i>	514	9	09/20/96

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													Yes	No
JB		0	0	5	7	3	0	9	09/28/00	PCT				
JB		9	7	2	7	3	1	9	07/31/97	PCT				
JB		9	7	2	7	4	8	0	07/31/97	PCT				
JB		9	9	0	6	5	9	7	02/11/99	PCT				

OTHER ART (Including Author, Title, Date, Pertinent Pages, Etc.)

not considered	✓	3D QSAR in Drug Design Kubinyi, H (ed.) Kluwer Academic Publishers (1993). <i>no copy provided</i>
JB	✓	Abagyan <i>et al.</i> Biased Probability Monte Carlo Conformational Searches and Electrostatic Calculations for Peptides and Proteins, <i>J. Mol. Biol.</i> <u>235</u> : 983-1002 (1994).
	✓	Abagyan <i>et al.</i> Protein structure prediction by global energy optimization, <i>Comput. Simul. Biomol. Syst.</i> 3:363-94 (1997).
*		Ajay <i>et al.</i> , Computational Methods to Predict Binding Free Energy in Ligand-Receptor Complexes, <i>Journal of Medicinal Chemistry</i> , 38(26):4953-4967 (1995).
	✓	Altschul, Gap costs for multiple sequence alignment, <i>J. Theor. Biol.</i> , 138:297-309 (1989)
	✓	Altschul and Lipman, Trees, stars and multiple biological sequence alignment, <i>SIAM J. Appl. Math.</i> , 49:197-209 (1989)
	✓	Altschul, Leaf pairs and tree dissections, <i>SIAM J. Discrete Math.</i> , 2:293-299 (1989)
	✓	Altschul <i>et al.</i> , Weights for data related by a tree, <i>J. Molec. Biol.</i> , 207:647-653 (1989)
	✓	Altschul <i>et al.</i> Basic Local Alignment Search Tool, <i>J. Mol. Biol.</i> <u>215</u> : 403-10 (1990).
*		Balaji <i>et al.</i> , Conformational studies on model peptides with 1-aminocyclopropane 1-carboxylic acid residues, <i>Pept. Res.</i> 7(2):60-71 (1994).
*		Balaji <i>et al.</i> , Conformational studies on model peptides with 1-aminocyclobutane 1-carboxylic acid residues, <i>Pept. Res.</i> 8(3):178-86 (1995).
*		Balasubramaniam <i>et al.</i> , [D-TRP ³²]Neuropeptide Y: A Competitive Antagonist of NPY in Rat Hypothalamus, <i>J. Med. Chem.</i> 37(6):811-815 (1994).
	✓	Balasubramanian, R., New type of representation for mapping chain-folding in protein molecules, <i>Nature</i> <u>266</u> : 856-57 (1977).
	✓	Bernstein <i>et al.</i> , The protein data bank: a computer-based archival file for macromolecule structures, <i>J. Mol. Biol.</i> , 112:535-542 (1977)

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OTHER ART (Including Author, Title, Date, Pertinent Pages, Etc.)

not considered	✓	Biocomputing: Informatics and Genome Projects Smith, D.W., ed. Academic Press, Inc., San Diego (1994). <i>no copy provided</i>
* JB		Böhm, Prediction of binding constants of protein ligands: A fast method for the prioritization of hits obtained from de novo design or 3D database search programs, <i>Journal of Computer-Aided Molecular Design</i> , 12:309-323 (1998).
	✓	Bouras <i>et al.</i> Design, Synthesis, and Evaluation of Conformationally Constrained Tongs, New Inhibitors of HIV-1 Protease Dimerization, <i>J. Med. Chem.</i> 42: 957-62 (1999).
	✓	Carrillo, H. and D. Lipman., The Multiple Sequence Alignment Problem in Biology, <i>SIAM J. Appl. Math.</i> 48(5): 1073-82 (1988).
	✓	Carson and Bugg, Algorithm for ribbon models of proteins, <i>J. Mol. Graphics</i> , 4:121-122 (1986)
	✓	Carson, Ribbons 2.0, <i>J. Appl. Cryst.</i> , 24:958-961 (1991)
	✓	Carson, Ribbon models of macromolecules, <i>J. Mol. Graphics</i> , 5:103-106 (1987)
	✓	Carson, Ribbons, <i>Methods in Enzymology</i> , R.M. Sweet and C.W. Carter, eds, Academic Press, 277:493-505 (1997)
* ↓		Checa <i>et al.</i> , Assessment of Solvation Effects on Calculated Binding Affinity Differences: Trypsin Inhibition by Flavonoids as a Model System for Congeneric Series, <i>J. Med. Chem.</i> 40:4136-4145 (1997).
not considered	✓	Computational Molecular Biology: Sources and Methods for Sequence Analysis Lesk, A.M., ed. Oxford University Press, New York (1988) <i>no copy provided</i>
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